U.S. DEPARTMENT OF ENERGY

Nuclear Energy

Reprocessing Plant-Level Toolkit Architecture

Valmor de Almeida

Oak Ridge National Laboratory

NEAMS PI Meeting

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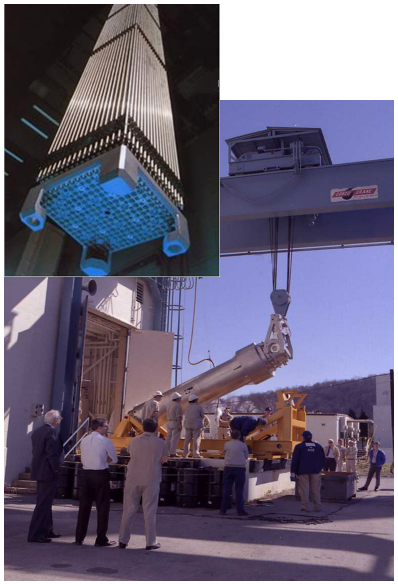
SafeSeps IPSC Toolkit

- **NEAMS Safeguards and Separations:** Develop a toolkit for realizing models of a modular reprocessing plant:
  - Generic; including aqueous, electrochemical, and alternative reprocessing methods.
  - Dynamic, coupled, hierarchical across physical scales, and extensible.
  - Safeguards by design.

Used Nuclear Fuel



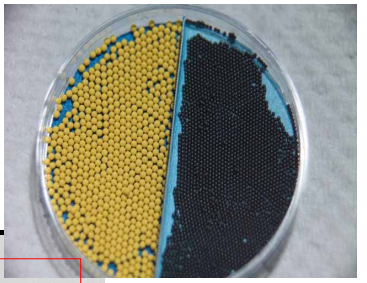
fuel receiving

Reprocessing Plant

- ***Numerous physico-chemical processes***

Safeguards by design

Product Forms



Fuel Fab

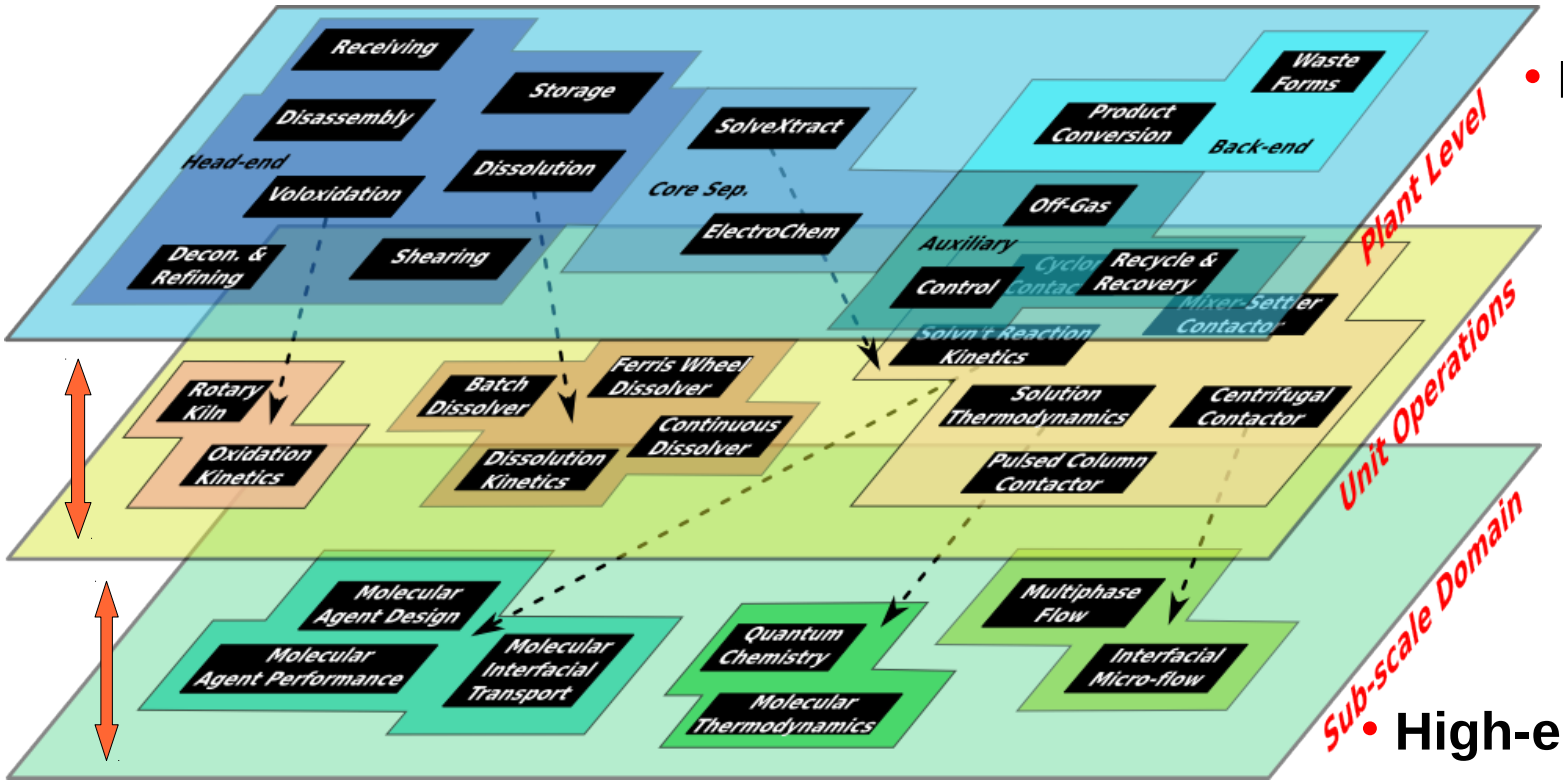
U/Pu/Np forms

Waste Disposal

Waste Forms

Nuclear Reprocessing Simulation Toolkit

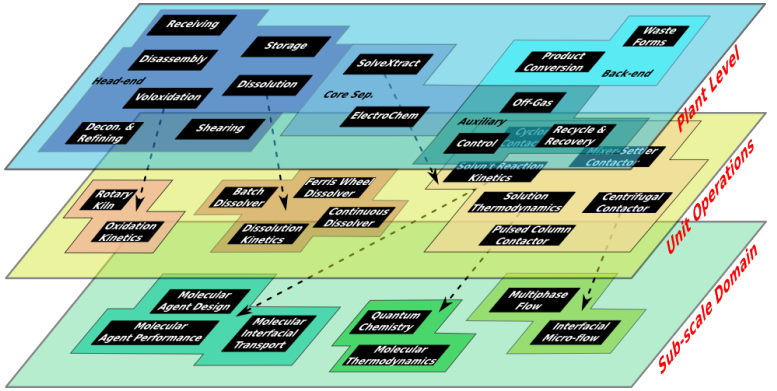
- **Multi-tiered approach**
  - **Plant-level:**
    - Low-order, time-dependent, tightly coupled, semi-empirical
  - **Unit Operations:**
    - Higher order, time-dependent, loosely coupled, continuum
  - **Sub-scale Domain:**
    - Electronic, atomistic, particle-based, structured continuum, stand-alone



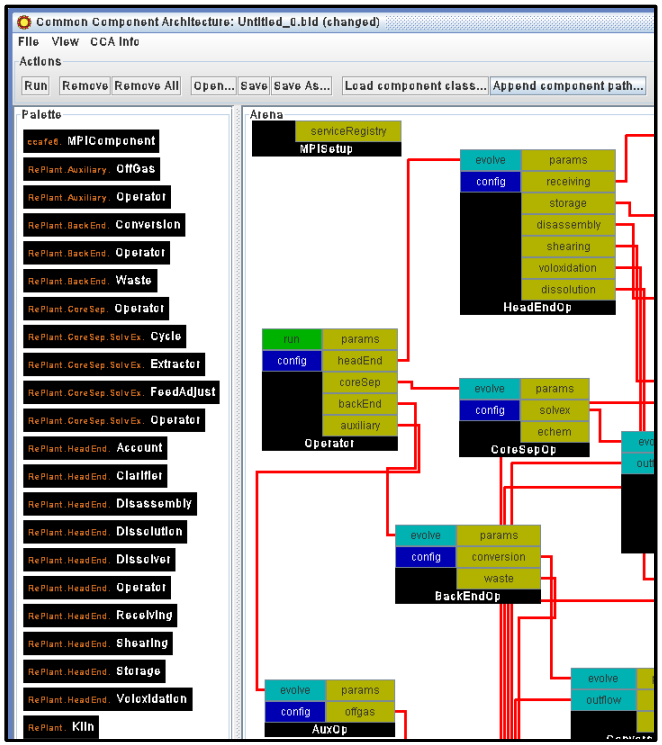
- **Desktop computing**
- **Cluster computing**
- **High-end parallel computing**

Multi-tiered Implementation

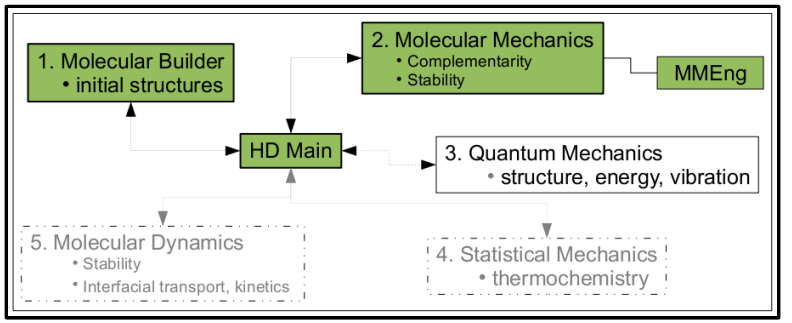
- **Multi-tiered implementation**
  - **Top-down:**
    - Plant-level components for all reprocessing processes
  - **Bottom-up:**
    - Prioritized processes that help users in the short-term

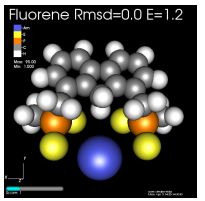


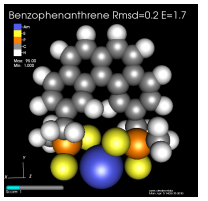
Plant-level

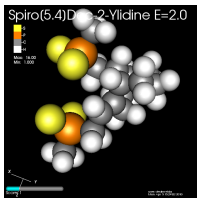


Solvent Extraction Agent Design







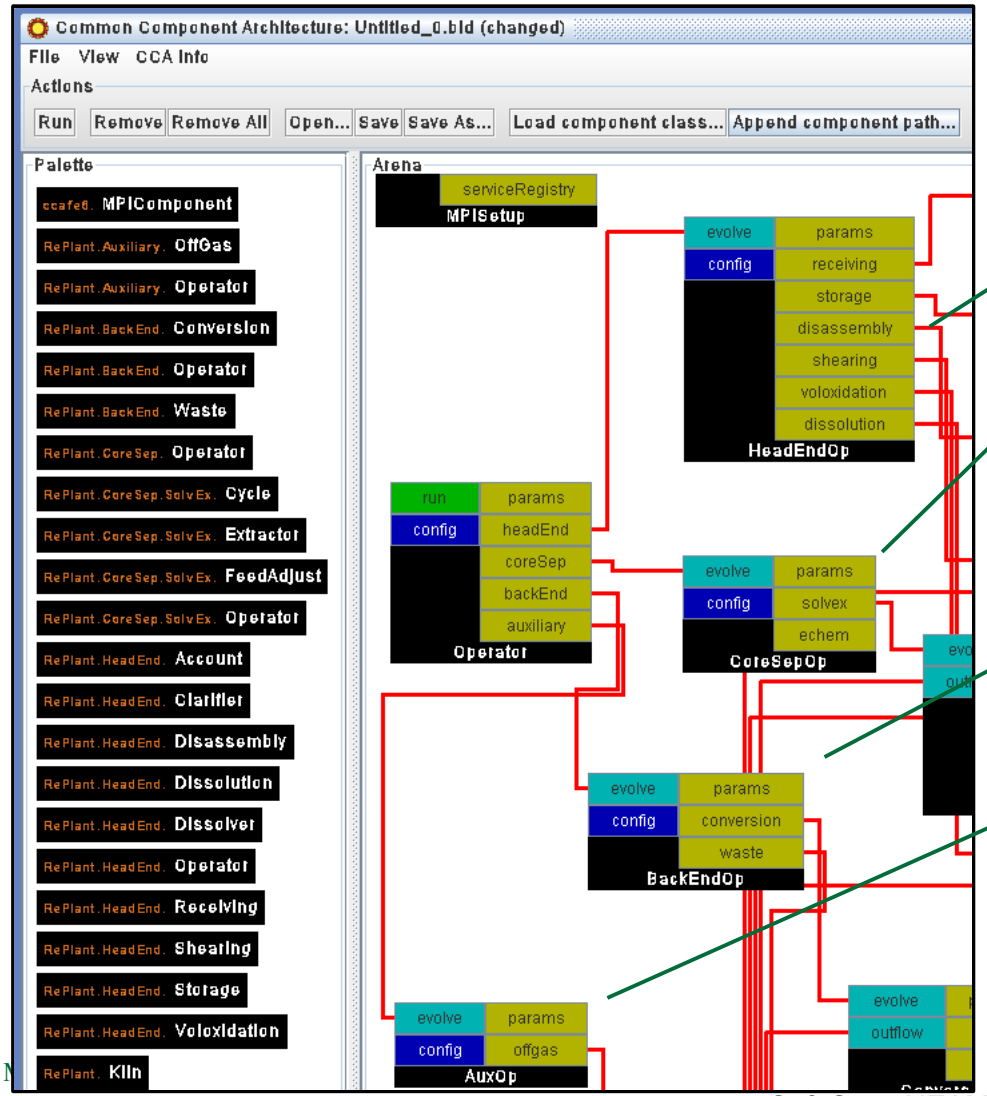


- NE Fuel Cycle R&D
  - Separations and waste forms technical area
  - Quantitative PIRT re-analysis

- Minor Actinides Separations Sigma Team
  - New ligands for Am/Cm separation

Plant-Level Toolkit Status

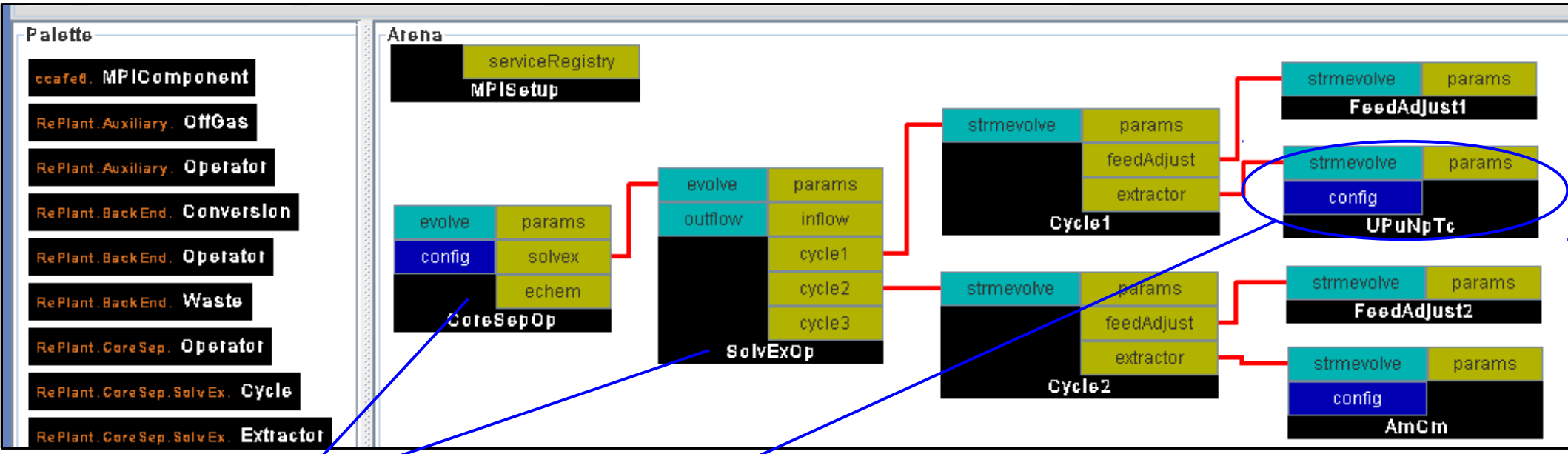
- **Using open source Common Component Architecture tools:**
  - Adopted the CCA specification
  - Used Ccaffeine framework to compose a plant-level application
  - Took advantage of Babel's language interoperability through SIDL
  - Adopted a library wrapping approach for existing plant-level codes
  - MPI-ready for testing in parallel



- **Sub-systems**
  - Head-End
    - Voloxidation
    - Dissolution
  - Core Separation
    - Aqueous based
      - Solvent extraction
    - Electrochemistry
  - Back-End
    - Conversion
    - Waste
  - Auxiliary
    - Off-gas

- **Material transport**
  - SIDL class for a stream
  - SIDL array of streams

Stand-alone Library Approach



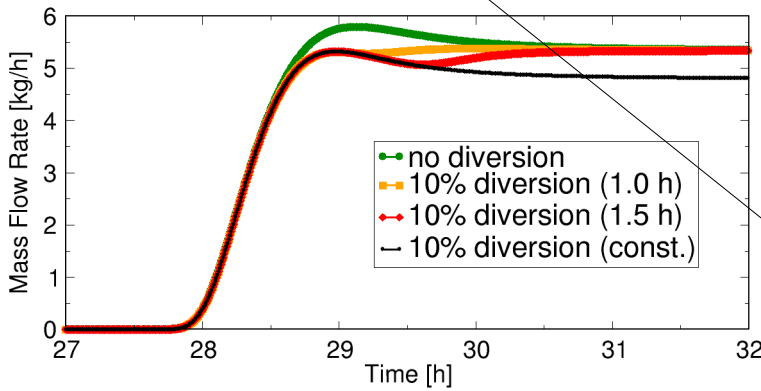
algorithm logic

library wrappers

underlying library

CCA components + Framework + Wrapped Libraries

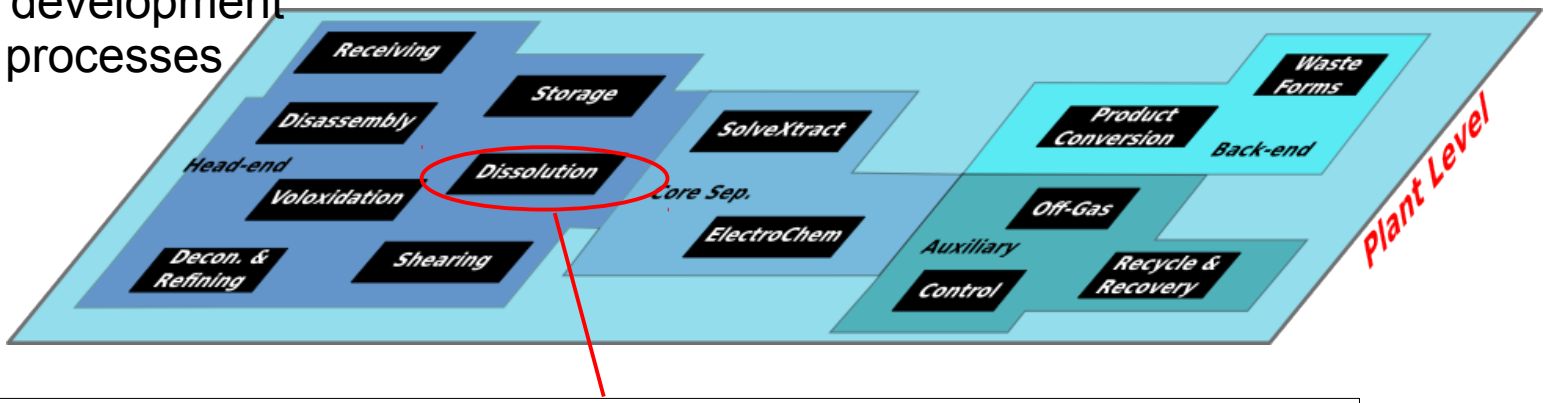
Solv. Extr. Contactor Bank



- Chemical Kinetics
- Mass and Energy Balance Module
- Distribution Coefficients
- Contactors

Plant Process Commonality

- **Chemical separation processes "architecture":**
  - Re-usable architecture will help guide modeling of different processes
  - Paves the way for incorporating sub-scale calibrations
  - Reduces time of code development
  - Applies to many plant processes



Mass & Energy Balance

Thermodynamics

extent of separation

- Phase equilibria

Contactors

mechanics of separation

- Multistage transport

Kinetics

speed of separation

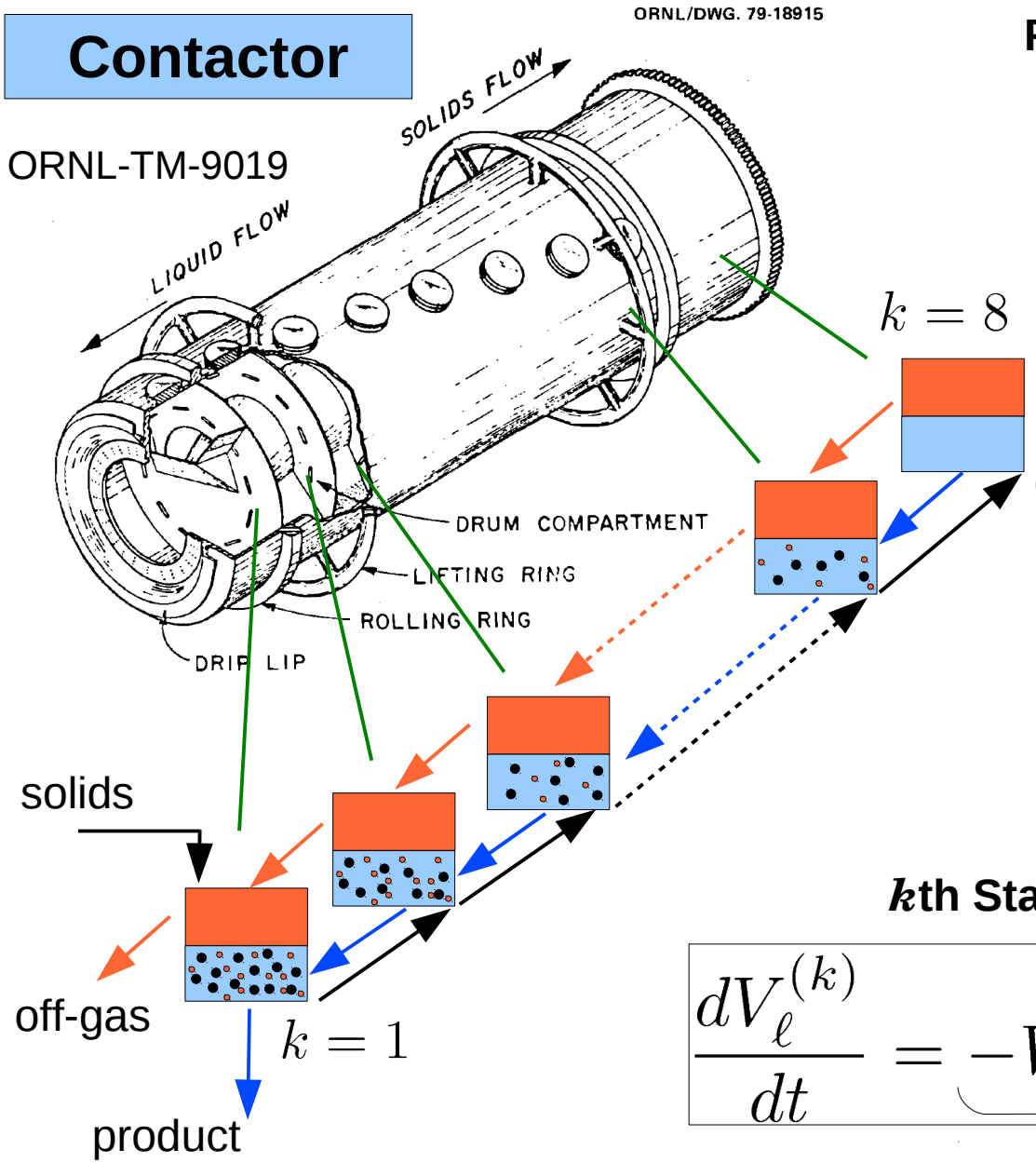
- Reaction mechanisms

Mathematical Problem → **Robust Solvers**

Fuel Dissolution Mechanics

Contactor

ORNL-TM-9019



Function
- Leach fuel in boiling HNO_3 aqueous stream
- Wash cladding
- "Accountability"

Materials
- **Feed:** solids, liquid, gas
- **Product:** liquid
- **Outflow:** off-gas, solids

Continuous Process
- Countercurrent (intermittent solid flow)
- Rotary dissolver

Prototype
- Rotary dissolver
- DOE Fuel Reprocessing Program 70-80's
- 0.5 ton/day HM full-scale ORNL

***k*th Stage "Volume Balance"**

$$\frac{dV_\ell^{(k)}}{dt} = \underbrace{-W(V_\ell^{(k)})}_{\text{experimentally measured (ORNL-TM-9019)}} + F^{k+1}$$

Additional Dissolution Components

Kinetics Overall reaction mechanism

$$UO_2(s) + 2.7\ HNO_3 \longrightarrow UO_2(NO_3)_2 + 0.7\ NO(g) + 1.3\ H_2O$$

$$K_{UO_2} = 0.480\ f\ [HNO_3]^2 \exp(-0.091\ T_d)$$

- f: surface roughness
- T_d: % of theoretical UO_2 density

experimental dissolution rate
ORNL-TM-3695

$$\dot{m}_{UO_2} = K^{(k)}_{UO_2}\ A_s$$

- A_s: surface area

Thermodynamics Non-ideal liquid solution

$$\rho_\ell^{(k)} = R(T, P, \rho^{(k)}_{H_2O}, \rho^{(k)}_{HNO_3}, \rho^{(k)}_{UO_2(NO_3)_2})$$

Mass & Energy Balance Mass balance for each specie:

$\rho_{UO_2(NO_3)_2}$
ρ_{HNO_3}
ρ_{H_2O}

$$\frac{d\,\rho_i^{(k)}}{dt}\ V_\ell^{(k)} + \rho_i^{(k)}\ \frac{dV_\ell^{(k)}}{dt} = -F^{(k)}\ \rho_i^{(k)} + S_i^{(k)}$$

ith species
kth stage

Common Computing Modules

Mathematical Problem

Non-linear DAE's

state vector

operation parameters

source parameters

$$\boldsymbol{G}\left(\frac{d\boldsymbol{x}}{dt}, \boldsymbol{x}, \boldsymbol{p}(t), \boldsymbol{q}(t)\right) = \boldsymbol{0}$$

Coupling of plant-level components are expressed mathematically as sources

Shearing

Dissolution

$$\boldsymbol{x}(0) = \boldsymbol{x}_0, \ \boldsymbol{p}(0) = \boldsymbol{p}_0, \ \boldsymbol{q}(0) = \boldsymbol{q}_0$$

$$\frac{d\boldsymbol{x}}{dt}(0) = \dot{\boldsymbol{x}}_0$$

Consistent initial conditions

Robust Solvers

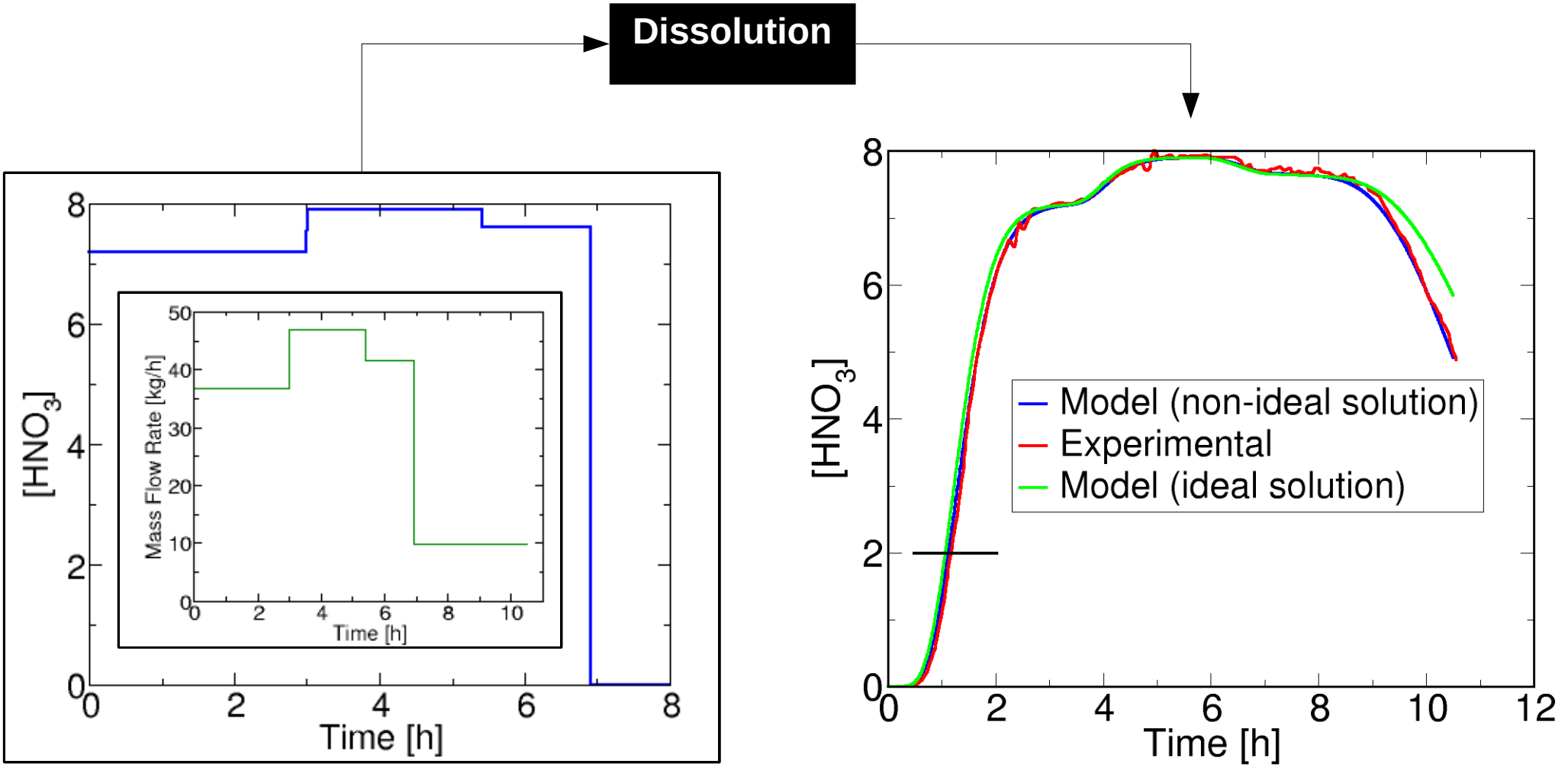
DASPK, DASPKSO, and others (including parallel versions)

- **It is advantageous to work with the naturally occurring equations**

Experimental Validation

- Liquid flow simulation with upstream upset

ORNL-TM-9019



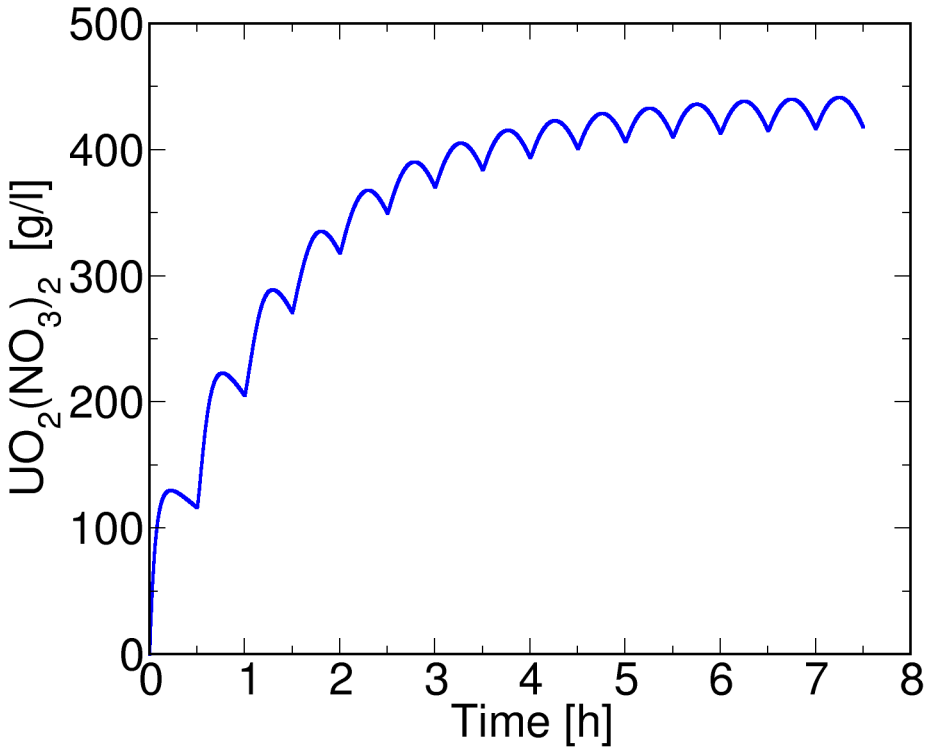
- At 2 Molar, non-ideal liquid solution differs 3.4 min. from experiments (ideal solution 7 min.)

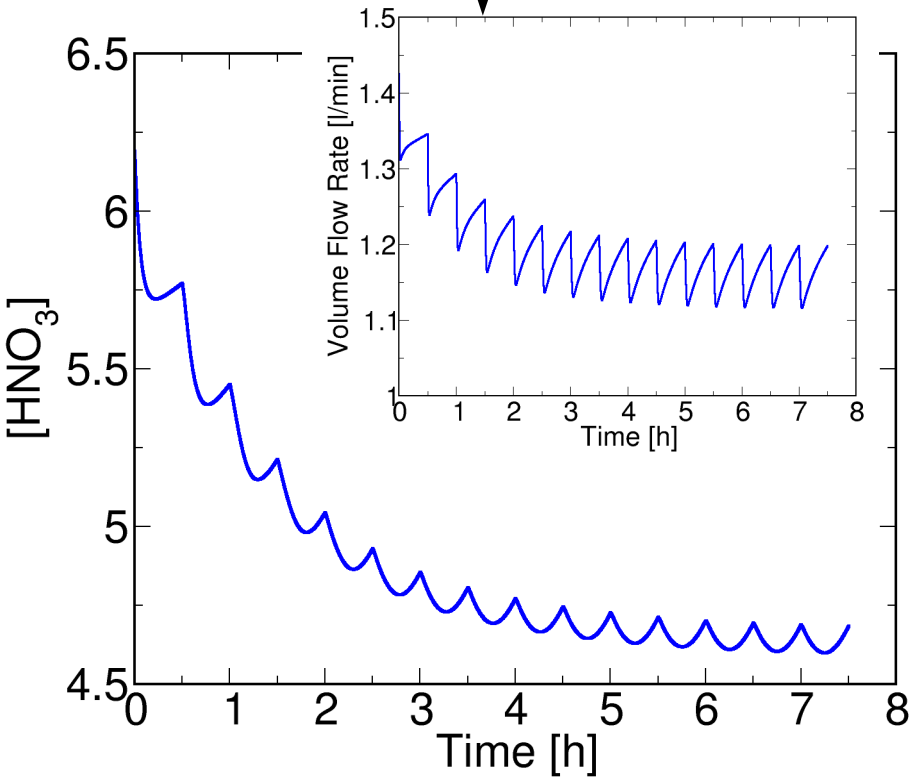
Additional Results

Shearing → **Dissolution**

- Product with suspended UO_2 particles (<10 µm diameter)

- **Feed:** UO_2 pellets (0.5 cm diameter)
- **Cycle:** 30 minutes
- **Capacity:** 0.5 t/day





➢ Not validated; input data based on ORNL-TM-9019

Path Forward

- **Toolkit challenge problem PUREX process demonstration in FY11:**
  - Extend dissolution component to include fission products and off-gas.
  - Extend dissolution subsystem to include digester tanks and accountability tank
  - Extend solvent extraction component to include pulse column and centrifugal contactors.

- **Model Driven System Development framework for the toolkit:**
  - CCA tools are currently unsupported.
  - MDSD usage-driven system design is a better fit for the user community and stakeholders.
  - Joint development with NEAMS ECT crosscut toward Version 0.9 in FY12.